Programming model and application porting to the Dynamical Exascale Entry Platform (DEEP)

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Outline

- DEEP Architecture
- Programming Model
- Applications
  - Climate Simulation (CYI)
  - CFD (CERFACS)
  - Superconductivity (CINECA)
- Conclusions

Credit where credit is due

- DEEP is a collaborative effort with contribution from many partners
- Contribution to the work here presented
  - Jülich Supercomputing Centre
  - University of Heidelberg/EXTOLL
  - Par-Tec
  - Barcelona Supercomputing Centre
  - Cyprus Institute
  - CERFACS
  - CINECA

DEEP Architecture

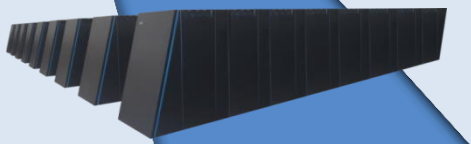
Constellation Systems

Intel Cluster Systems
(Juropa)

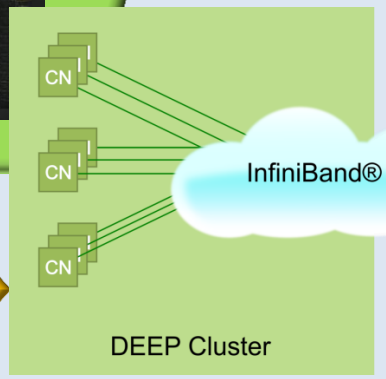
Graphic-card
Accelerated
Clusters

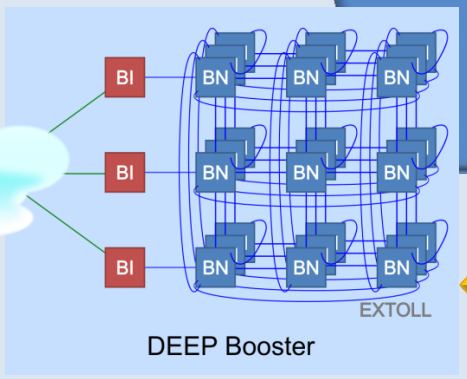
IBM Blue Gene/L

IBM Blue Gene/P



IBM Blue Gene/Q





HPC Cluster Architectures

Extremely Scalable Architectures

DEEP Architecture

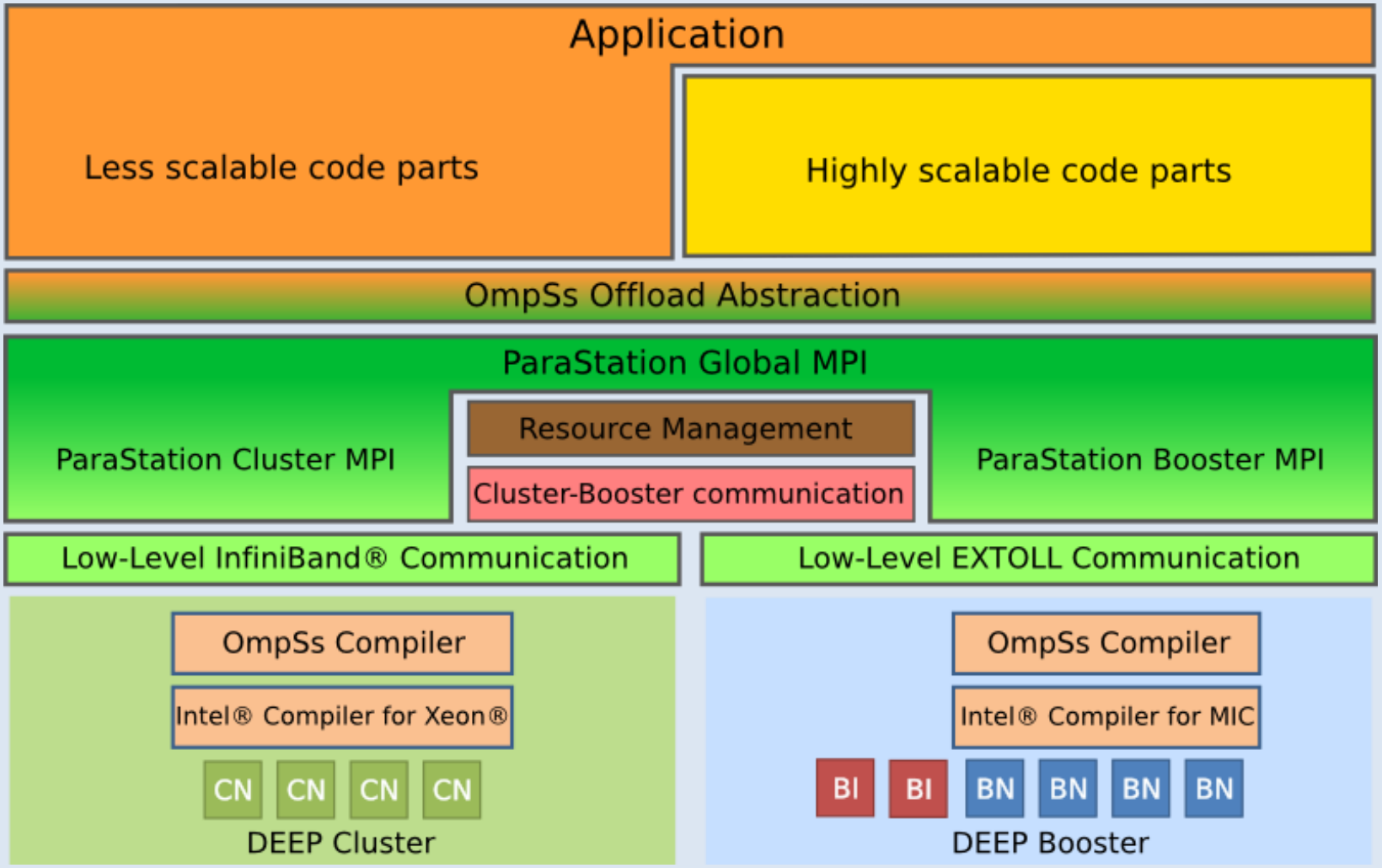
- Cluster Nodes
  - 128 Nodes
  - 2x Sandy Bridge processors
  - InfiniBand network
    - Fat tree
  - Connected to I/O
- Booster Nodes
  - 512 Nodes
  - 1x Xeon Phi
  - EXTOLL network
    - 3D torus
- Cluster-Booster Interface Nodes
  - 32 Nodes
  - InfiniBand and EXTOLL

DEEP Architecture

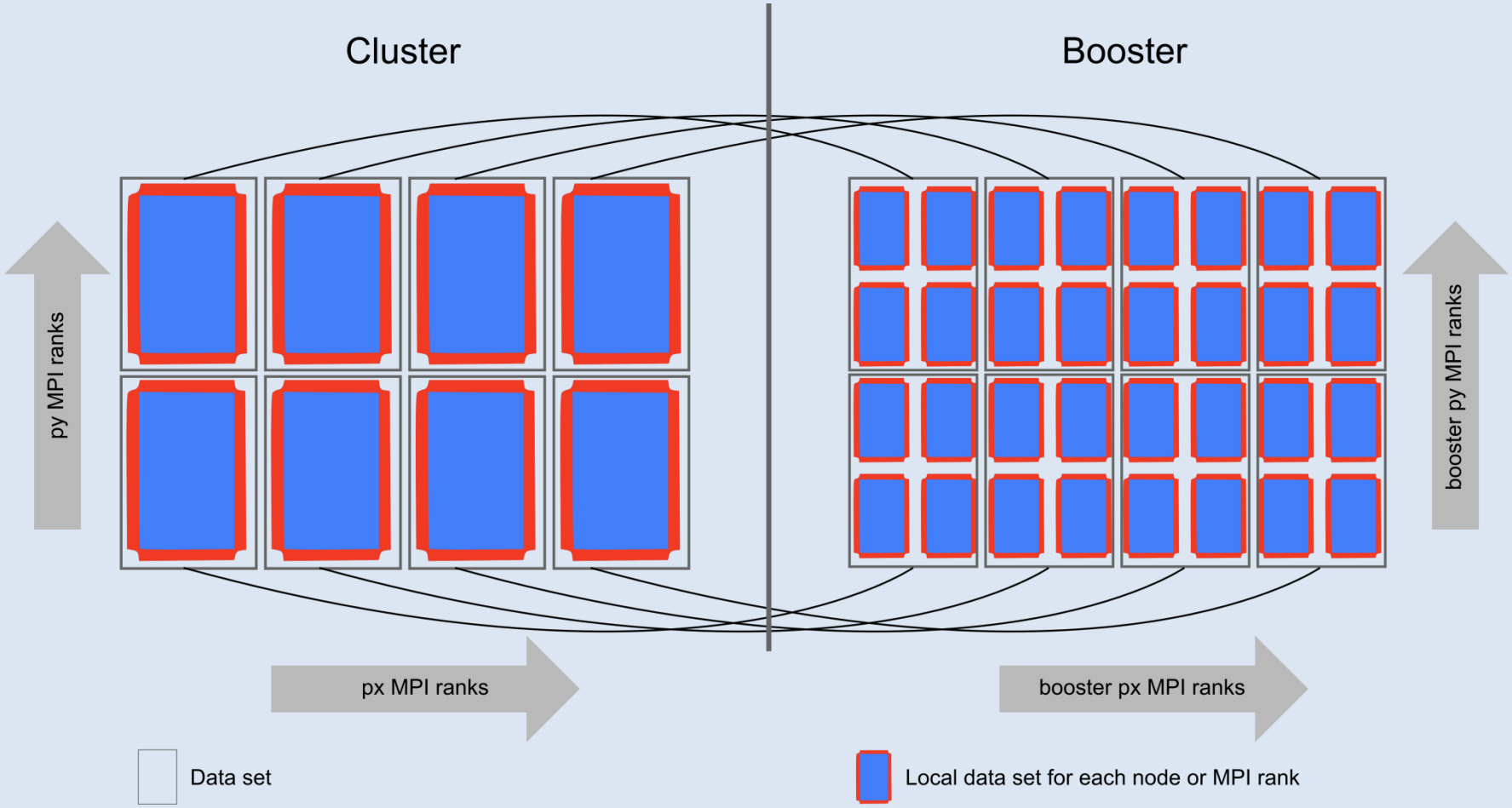
Technology	Implementation	Internal Clock Frequency	Link Bandwidth [Gb/s]	Latency [µs]	Effective maximum Bandwidth [GB/s]	Message Rate [msg/s]
EXTOLL VENTOUX	Xilinx Virtex6 FPGA	200 MHz	16 Gb/s	1.2 µs	Up to 1.4 GB/s	~ 25 millions
EXTOLL TOURMALET	65 nm ASIC	750 MHz	120 Gb/s	0.6 µs	Up to 10 GB/s	~ 100 millions
IB FDR*	45 nm ASIC	Unknown	56 Gb/s	0.8 µs	Not measured	Not measured
Typical 1GE	ASIC based	e.g. 125 MHz	1 Gb/s	e.g. 40 µs	0.11 GB/s	~0.5 millions
10GE	ASIC based	~125 to 312 MHz	12,5 Gb/s	12.5 µs	1.2 GB/s	< 2.5 millions
Cray Gemini	90 nm ASIC	650/800 MHz	75 Gb/s	1.5 µs	Up to 5.9 GB/s	~ 2 millions
Tianhe-1a	ASIC based	Unknown	80 Gb/s	2.5 µs	Up to 6.34 GB/s	~ 1-3 millions
TOFU (K-Computer)	65 nm ASIC	312.5 MHz	50 Gb/s	1.5 µs	Up to 4.76 GB/s	> 8 millions

* Mellanox literature data

Programming Model

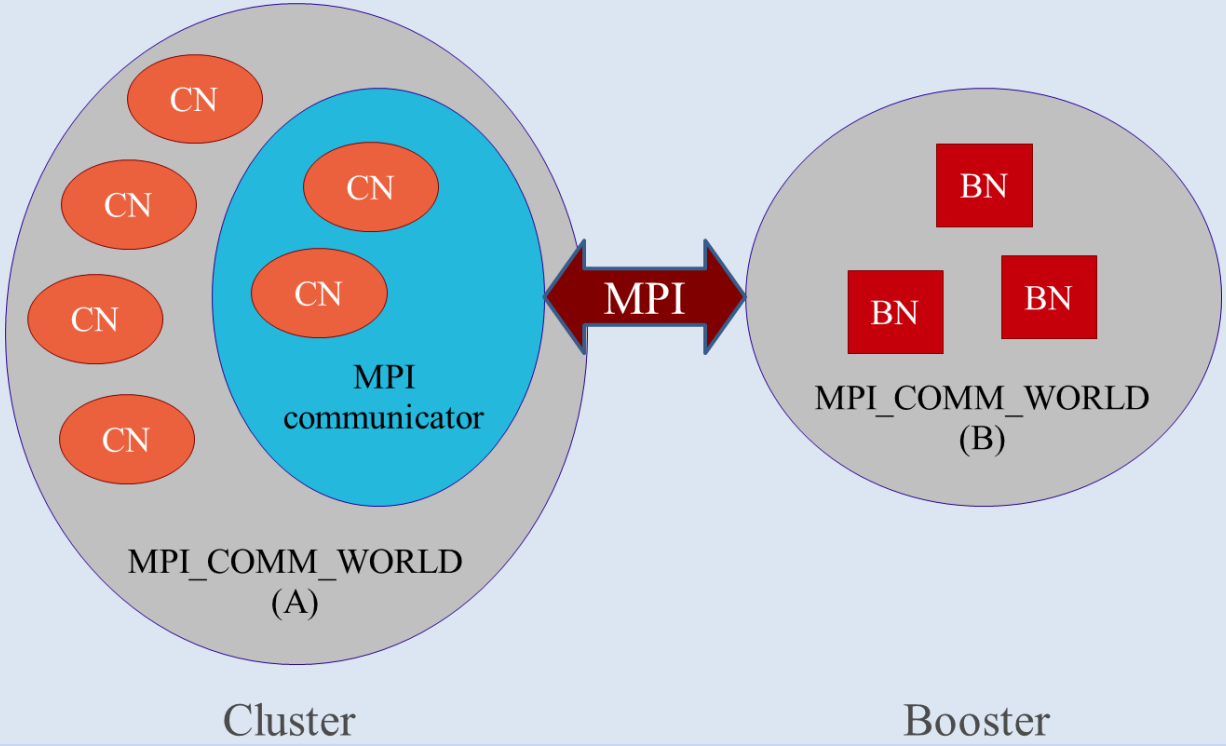


Programming Model



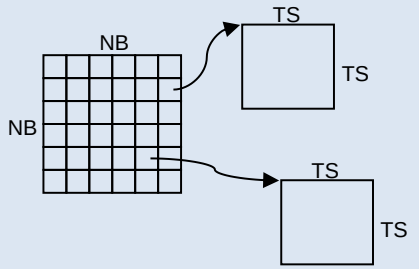
Programming Model

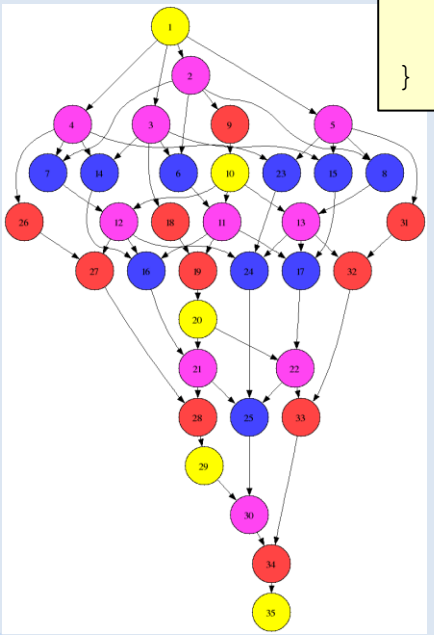
- "Global MPI"
  - Connect Cluster MPI and Booster MPI via MPI_Comm_spawn ()
  - Startup mechanism for Booster code parts
  - P2P communication mechanism via intercommunicator



Programming Model

```
void Cholesky( float *A[NT] ) {
int i, j, k;
for (k=0; k<NT; k++) {
   spotrf (A[k][k]) ;
   for (i=k+1; i<NT; i++)
      strsm (A[k][k], A[k][i]);
   for (i=k+1; i<NT; i++) {
      for (j=k+1; j<i; j++)
         sgemm( A[k][i], A[k][j], A[j][i]);
      ssyrk (A[k][i], A[i][i]);
   }
}
```



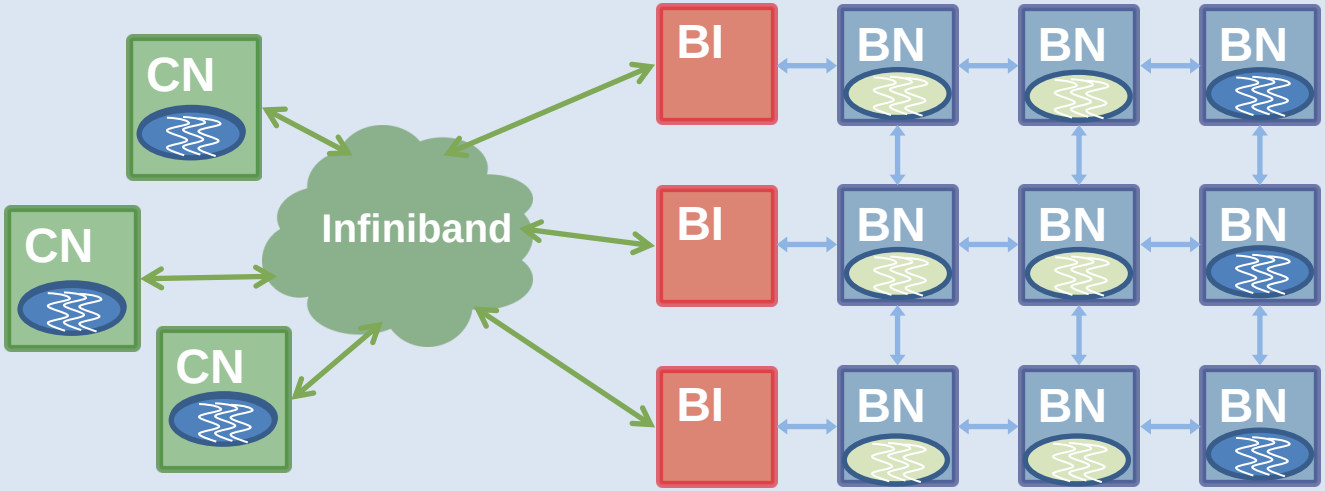


```
#pragma omp task inout ([TS][TS]A)
void spotrf (float *A);
#pragma omp task input ([TS][TS]T) inout ([TS][TS]B)
void strsm (float *T, float *B);
#pragma omp task input ([TS][TS]A,[TS][TS]B) inout ([TS][TS]C)
void sgemm (float *A, float *B, float *C);
#pragma omp task input ([TS][TS]A) inout ([TS][TS]C)
void ssyrk (float *A, float *C);
```

Decouple how we write (think sequential) from how it is executed

Programming Model

- Approach
  - MPI+OpenMP/OmpSs @ Cluster
  - MPI+OpenMP/OmpSs @ Booster
  - MPI+OpenMP/OmpSs @ whole System (Global MPI)



Programming Model

- “Collective” offload approach
  - Collective allocation of Booster Nodes
    - Define resources and communication name space

```
int DEEP_Booster_alloc( MPI_Comm cluster_comm,
                        int booster_nodes, ...,
                       MPI_Comm *intercomm);
```

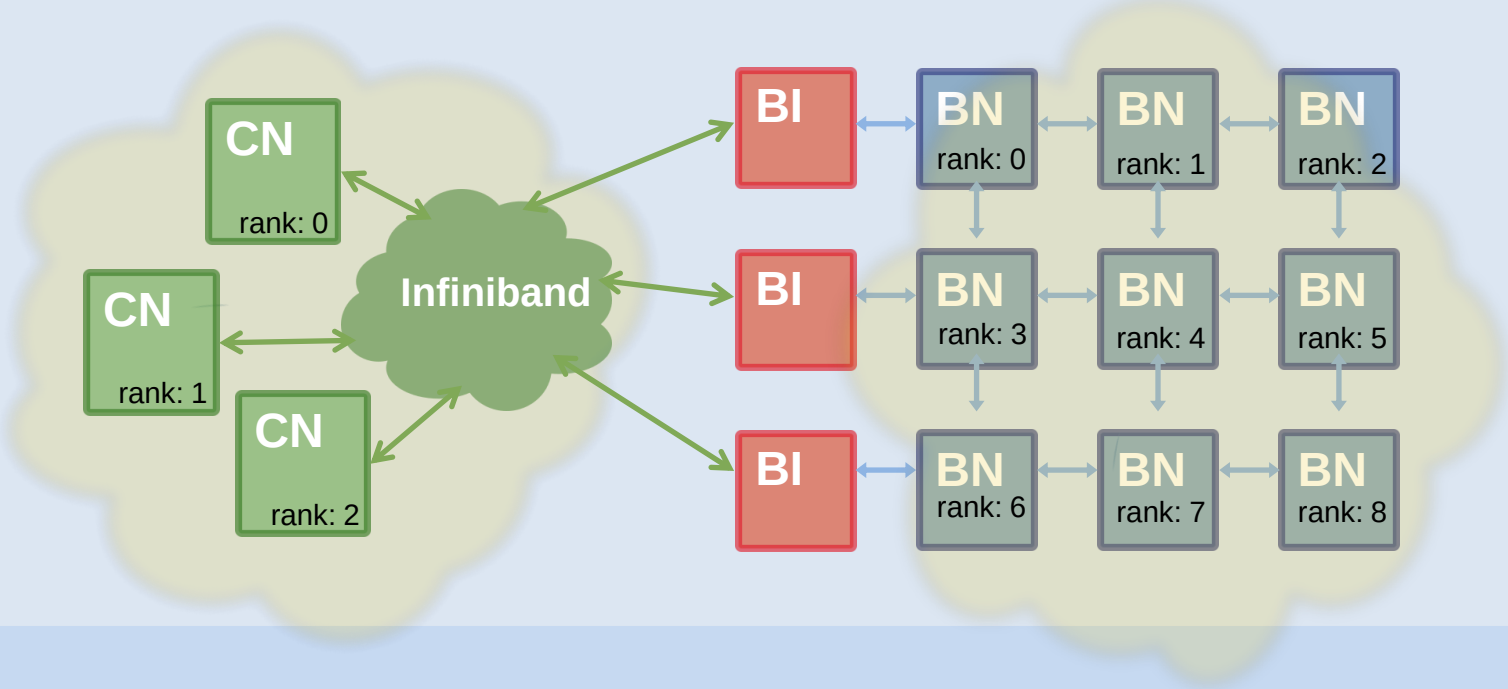
  - User controlled placement of tasks
    - Tasks can use MPI between them within allocated communicator

```
# pragma omp target device (intercomm:rank)
```

  - Standard MPI and OmpSs elsewhere
    - i.e.: CN ↔ BN transfers are asynchrony handled by standard OmpSs

Programming Model

```
int main(int argc, char *argv[]){
  MPI_Init(…);MPI_Comm_rank(…);MPI_Comm_size(…);
  MPI_Comm comm;
  DEEP_Booster_alloc(MPI_COMM_WORLD, size*3, size*3,
                     &comm);
  for(int i=0; i<3; i++){
    #pragma target device (comm:size*rank+i) copy_deps
    #pragma omp task input(…) output(…)
    foo_mpi(i,…);
  }
}
```



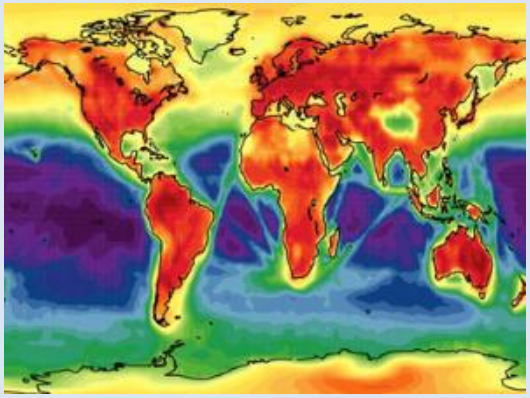
Programming Model

- Top-Level abstraction: OmpSs
  - **Hide the implementation details** from the application developer
  - Developer **annotates** the code to specify offloading semantics
- OmpSs allows to specify …
  - Booster topology (torus or grid, size)
  - Data distribution
- OmpSs compiler
  - Reads annotations, generates code calling the runtime
  - Generates (separate) executables for Cluster and Booster
- OmpSs runtime
  - Initiates kernels in the Booster
  - Handles data transfer between Cluster and Booster

Applications

- Climate Simulation (CYI)
- Computational Fluid Dynamics (CERFACS)
- High Temperature Superconductivity (CINECA)
- Seismic Imaging (CGGVeritas)
- Space Weather (KULeuven)
- Brain Simulation (EPFL)

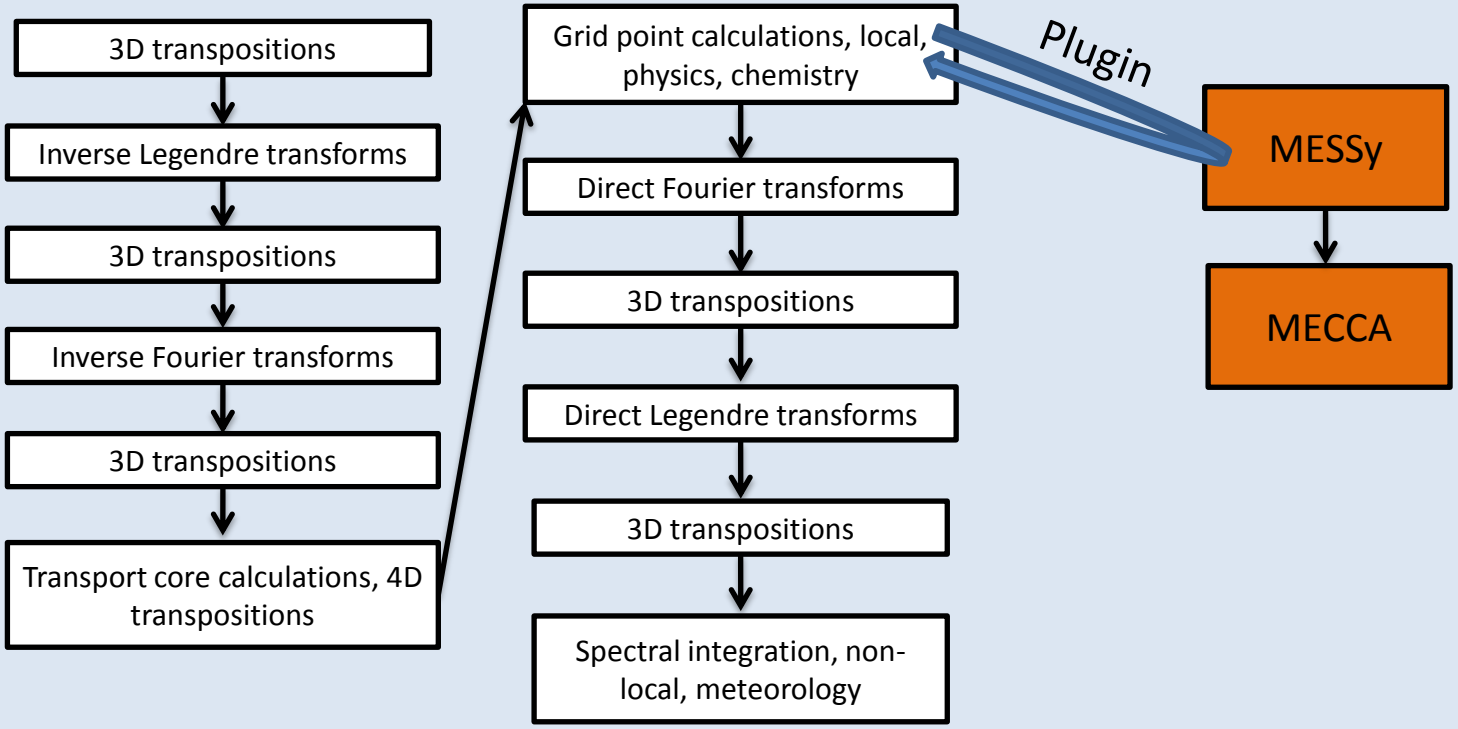
Climate Simulation (CYI)



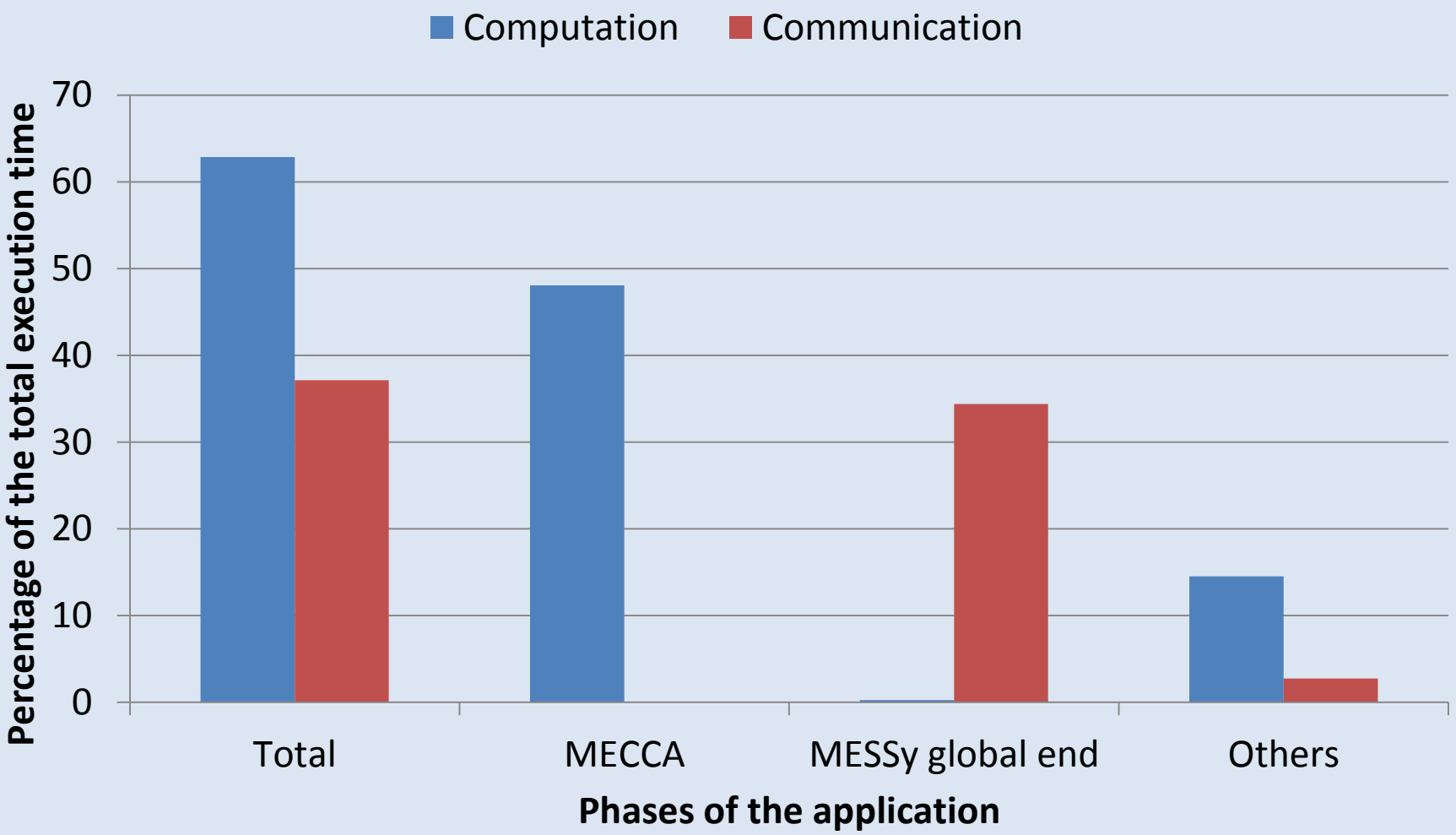
- Partner: CYI
- EMAC (ECHAM/MESSy Chemistry)
  - ECHAM provides a comprehensive general circulation model (GCM) of the atmosphere
  - MESSy (Modular Earth Submodel System) couples several physicochemical processes to it.
- Fortran 95

Climate Simulation (CYI)

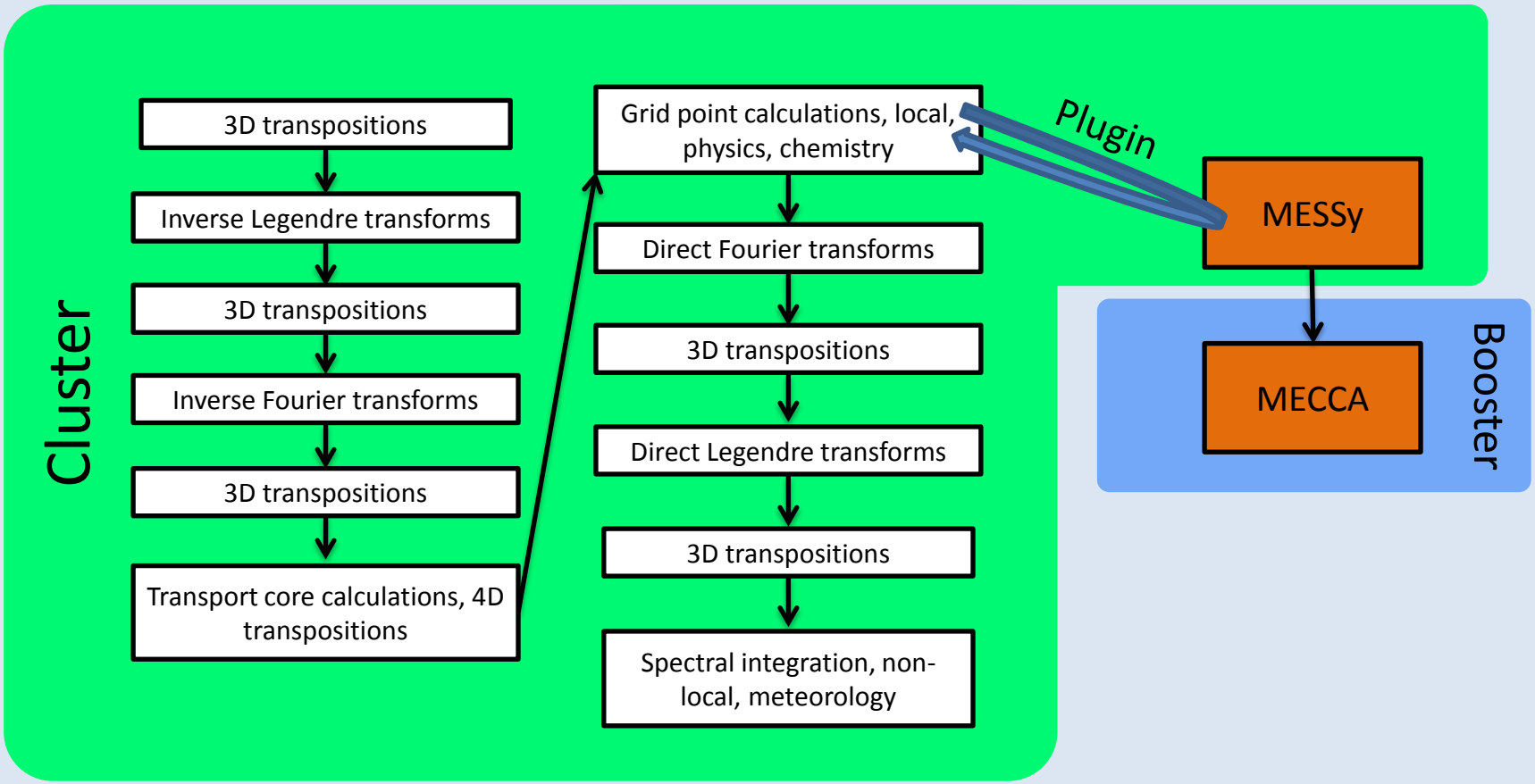
- Two coupled models:
  - ECHAM (Atmospheric)
  - MESSy (Physicochemical interactions)
  - EMAC = ECHAM/MESSy Atmospheric Chemistry



Climate Simulation (CYI)

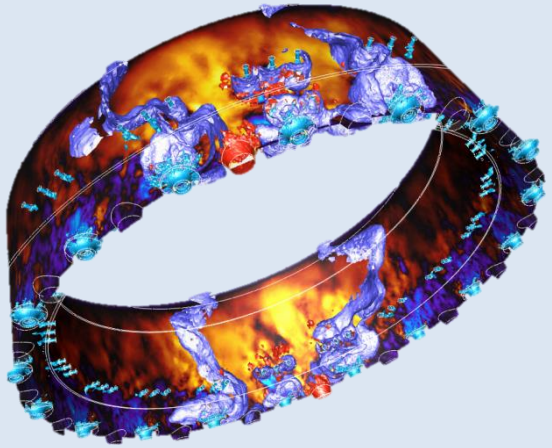


Climate Simulation (CYI)



CFD (CERFACS)

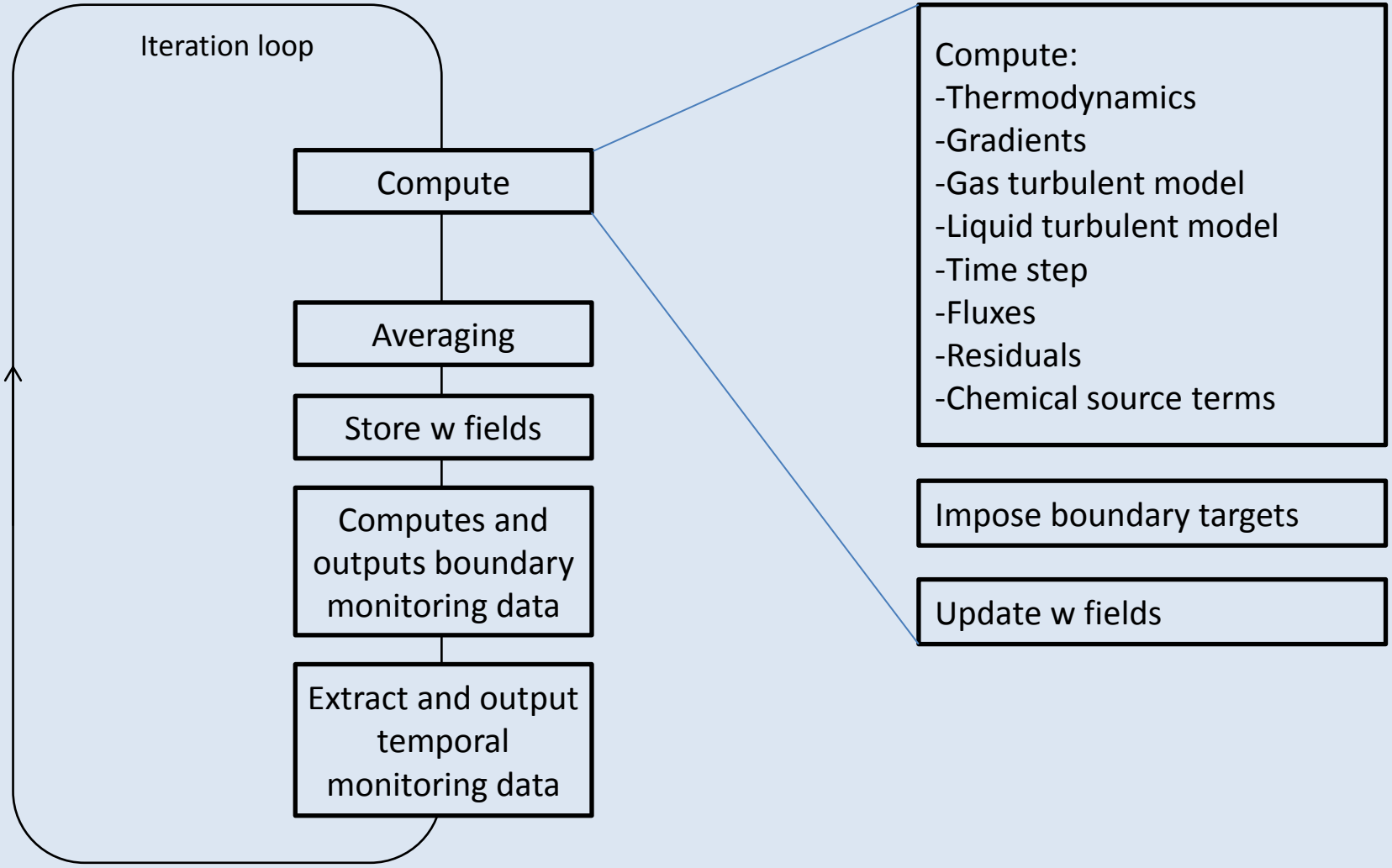
- Partner: CERFACS
- AVBP
- 3D Compressible Navier-Stokes solver
- Fortran + C



CFD (CERFACS)

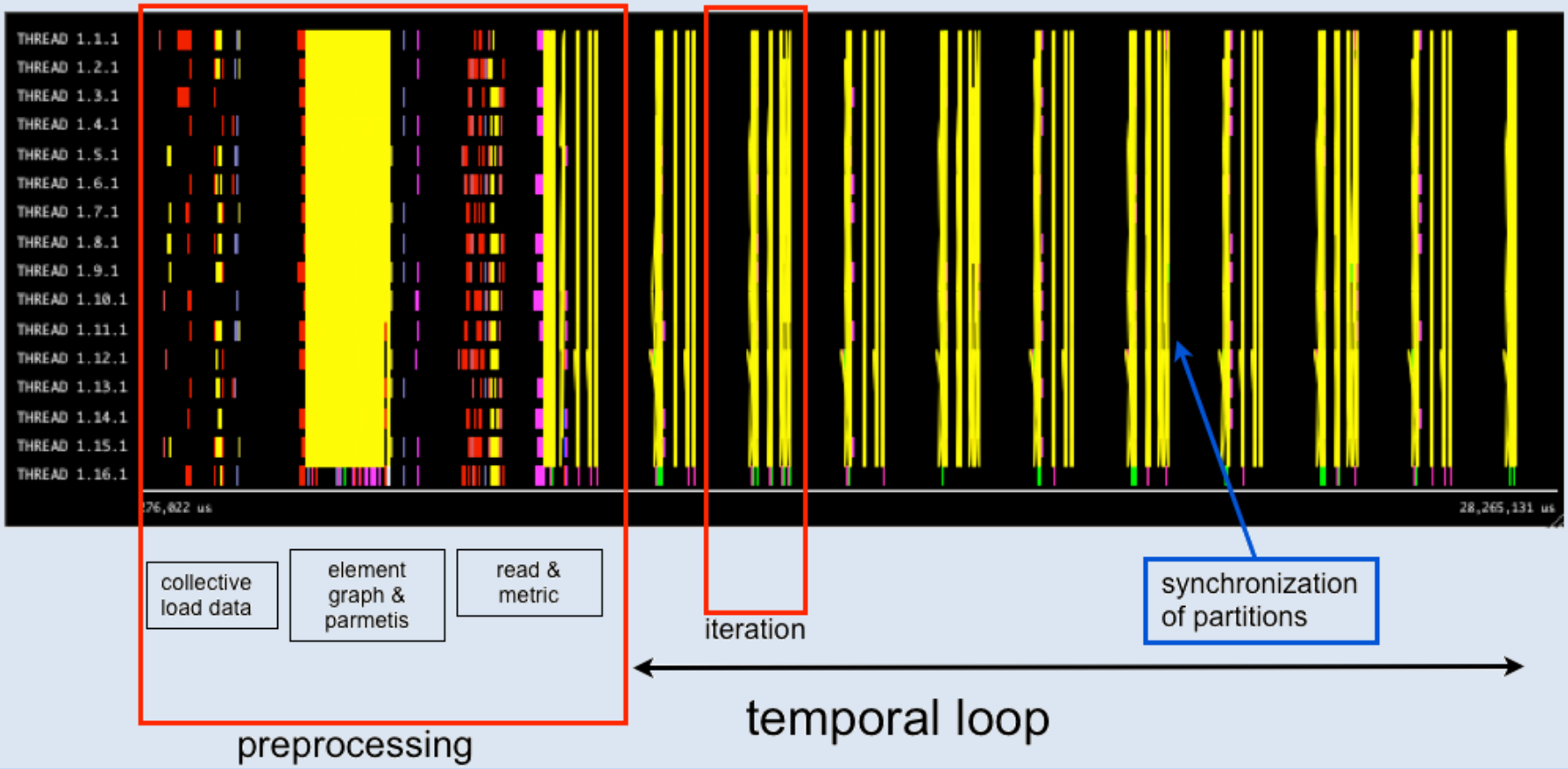
- Application structure
  - Phases
    - Read data
    - Decompose
    - Compute loop
      - Write snapshot every X cycles
  - The initial and I/O phases used to follow a master-slave approach
    - They have been optimized for scalability recently
  - Domain decomposition is done in parallel
  - I/O as well

CFD (CERFACS)


Iteration loop
Compute
Averaging
Store w fields
Computes and outputs boundary monitoring data
Extract and output temporal monitoring data
Compute:
-Thermodynamics
-Gradients
-Gas turbulent model
-Liquid turbulent model
-Time step
-Fluxes
-Residuals
-Chemical source terms
Impose boundary targets
Update w fields

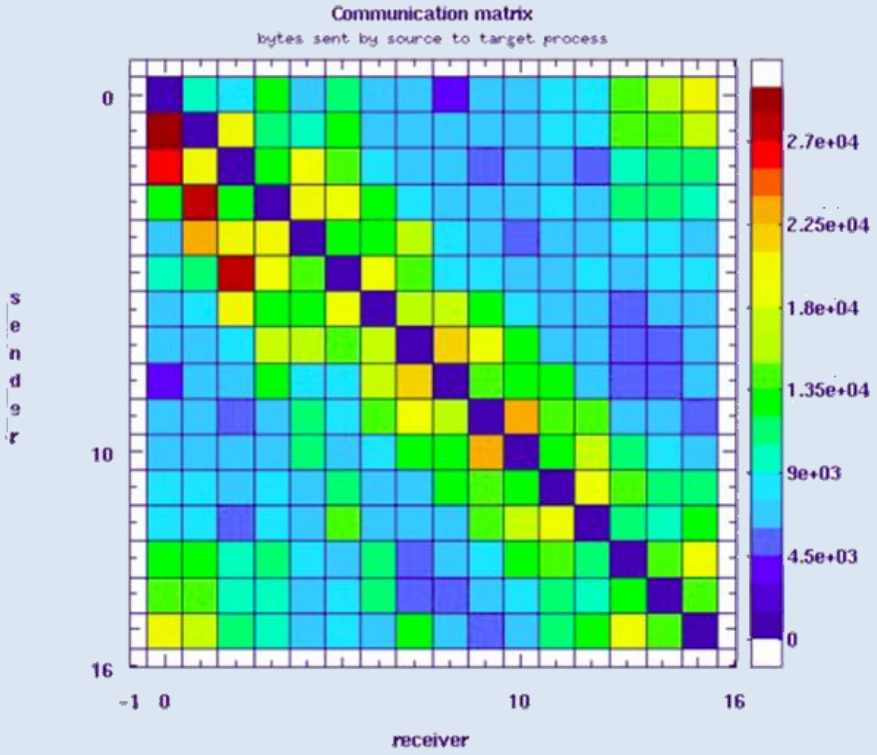
CFD (CERFACS)

- Trace of a 16 core simulation

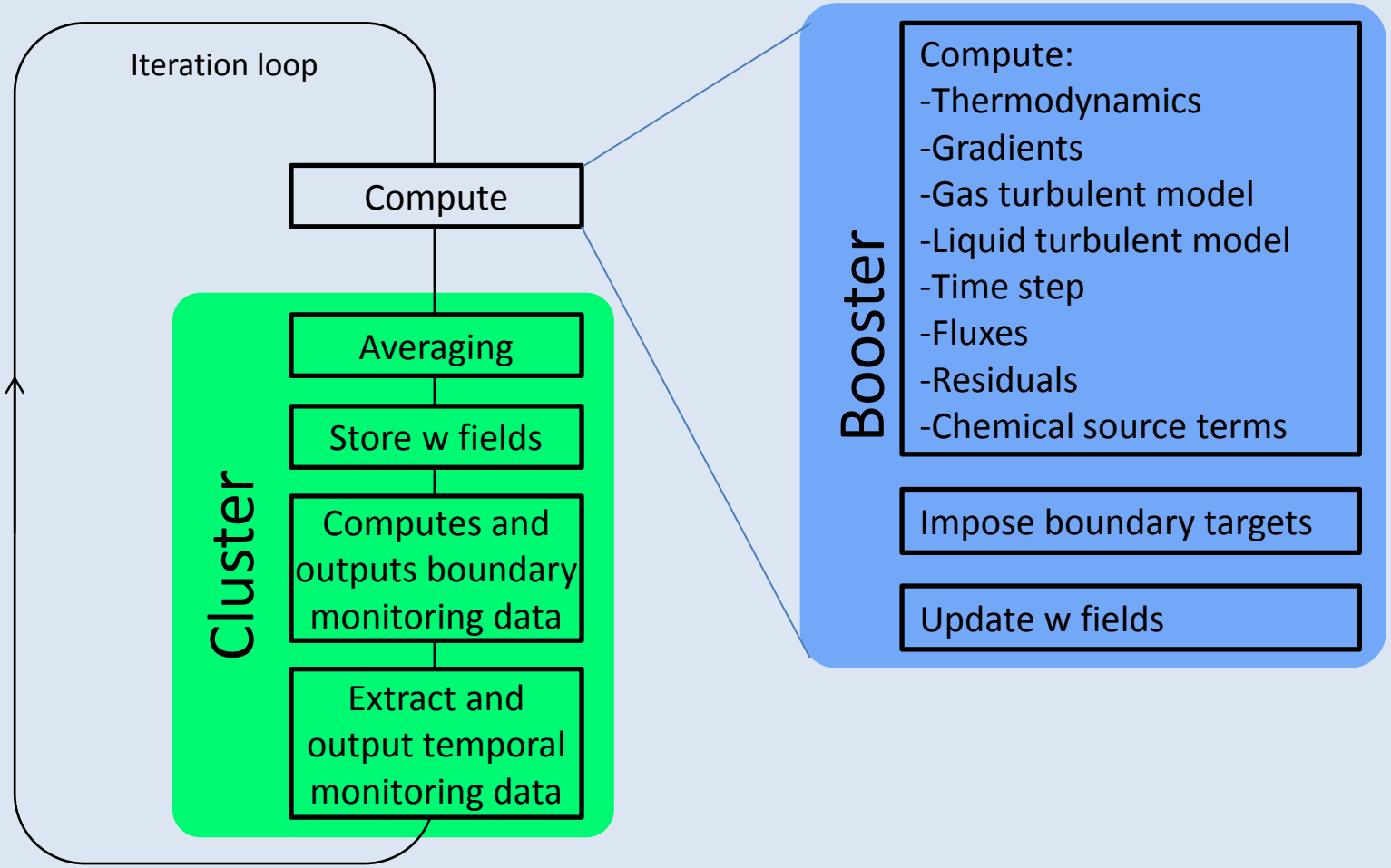


CFD (CERFACS)

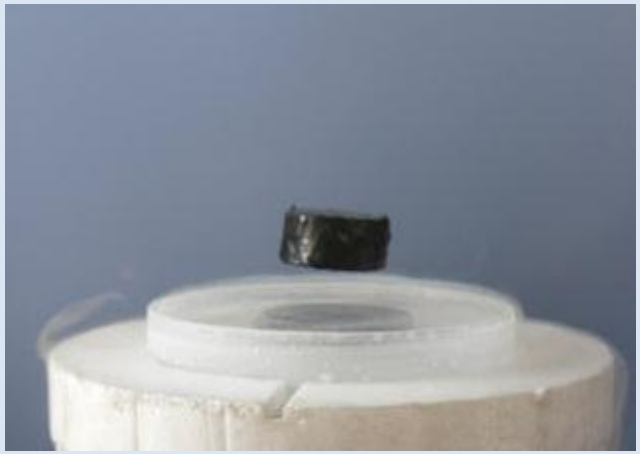
- Trace analysis (old version)
  - Computation takes ~50% of the time
  - Synchronization and boundary exchange takes ~20% of the time



CFD (CERFACS)


Iteration loop
Compute
Cluster
Averaging
Store w fields
Computes and outputs boundary monitoring data
Extract and output temporal monitoring data
Booster
Compute:
-Thermodynamics
-Gradients
-Gas turbulent model
-Liquid turbulent model
-Time step
-Fluxes
-Residuals
-Chemical source terms
Impose boundary targets
Update w fields

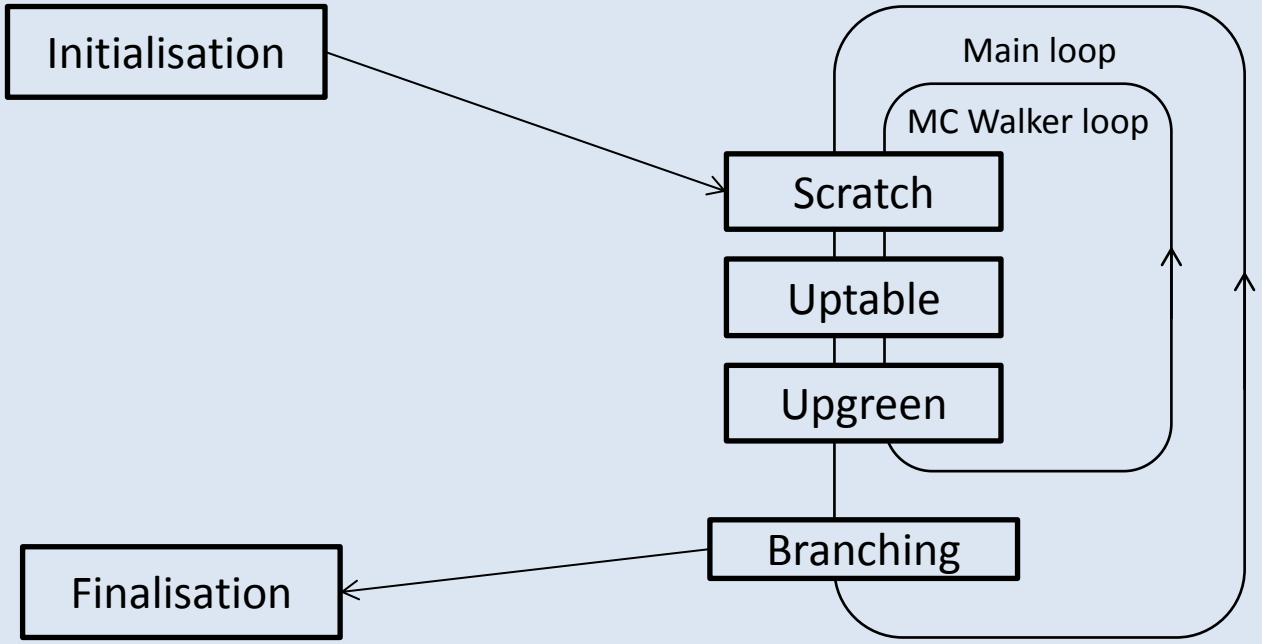
Superconductivity (CINECA)



- Partner: CINECA
- TurboRVB
- Quantum Monte Carlo simulations to study superconducting mechanisms in high critical temperature materials
- Fortran 90

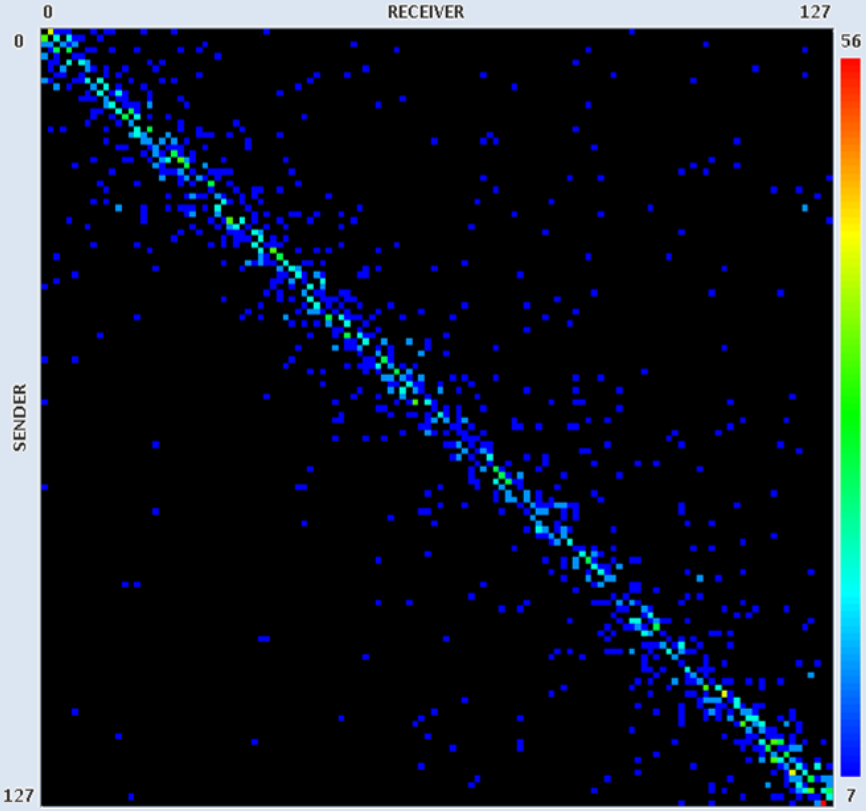
Superconductivity (CINECA)

- Phases:

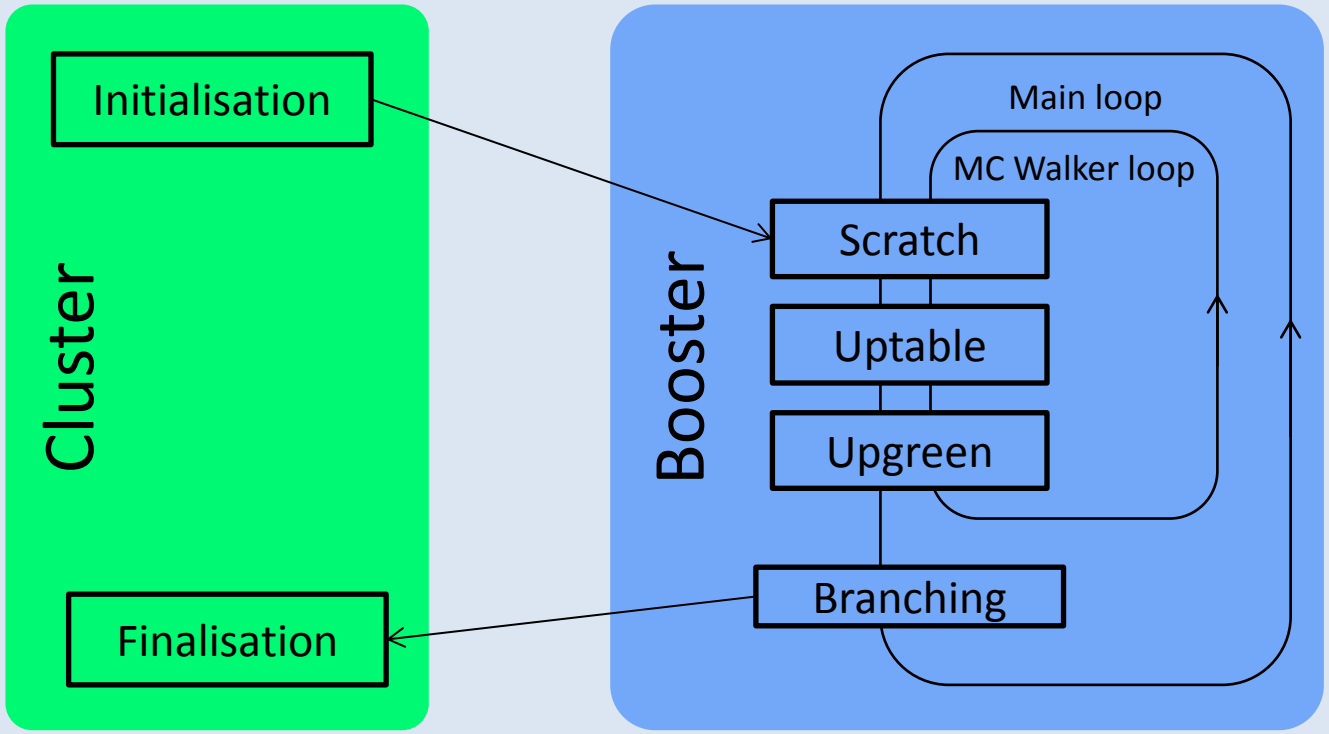


Superconductivity (CINECA)

- TAU communication matrix (number of calls)
  - Mainly nearest neighbours communication



Superconductivity (CINECA)



Conclusions

- DEEP provides a novel and flexible platform
- The programming model uses well known APIs
  - Plus a few changes to leverage asynchronicity and easy offloading
- Applications will be ported to it
  - Division between Cluster and Booster is clear now

Thank you